New Type of Thin Film Texture Observed

Electron Microscopy Confirms Unique Plane Alignment

A collaborative project between IBM Watson researchers and Eric Stach at the National Center for Electron Microscopy has discovered a new type of thin film texture. Coined "axiotaxy," this texture is characterized by the sharing of only one set of lattice spacings between the film and its growth substrate. A report of the work appeared recently in *Nature*.

Thin metal films play an important role in advanced semiconductor devices, and are used to interconnect device elements on the chip. Often, these metallic films are formed through solid-state reactions between a metallic element and the silicon itself, resulting in compounds known as metal silicides. One of the most fundamental structural properties of a metal silicide film is its "texture," the orientation of its individual grains with respect to the deposition substrate. Texture is known to strongly affect electronic and mechanical properties as well as the long term reliability of these interconnects. Three types of texture are commonly observed: random, where no single orientation is dominant; fiber-texture, where one orientation of the film grains is parallel to the growth direction, but the distribution is random about that direction; and epitaxial, where the film orientation is fixed in three dimensions with respect to the substrate.

Conventionally, texture is determined through the use of large area x-ray diffraction "pole figures"which depict the relative orientation of crystalline grains in a material In this work, researchers from IBM Watson Research Lab utilized pole figures obtained at the National Synchrotron Light source, where they have a dedicated beamline, to investigate the texture of several silicide thin films of the type used as electrical contact materials in integrated circuits. Surprisingly, in addition to evidence of conventional epitaxial texture, complex arcs of intensity in specific locations were seen. The geometrical signature of these arcs suggested that the film and substrate shared a common plane orientation, resulting from a lattice matching of just one plane between the two components. However, this fixes only one crystallographic direction of the film grains, and the presence of these arcs of intensity suggested that there was a non-random distribution of orientations about this plane—i.e. an unusual fiber texture.

High-resolution electron microscopy was required to confirm the existence of this new type of texture. These samples presented several particular microscopy challenges that required use of a unique microscope at the National Center for Electron Microscopy, the 800 kV Atomic Resolution Microscope. This microscope has sufficient point-to-point resolution (1.6 Å), sample tilting capabilities (± 45° along two orthogonal axes) and high voltage (for increased sample penetration of the strongly scattering nickel silicide layers) to produce atomic resolution images of these samples. Extensive microscopy confirmed the presence of both conventional epitaxial grains, as well as grains with the new "axiotaxy" texture.

Additionally, the microscopy showed that those grains with an axitaxial relationship showed strongly curved interfaces between the film and substrate. This observation gives insight into the physical origin of this unique crystallographic behavior. If there is nearly exact lattice matching between the film and substrate planes, the one-dimensional periodicity of the interface can be preserved independent of the curvature of the interface. If, however, the lattice matching is less than perfect, and interfacial curvature results in increasing mismatch with curvature, eventually leading to a breakdown in the possibility of plane alignment.

The appearance of axiotaxy was observed in many different thin film systems formed by solid-state reactions and appears to be a robust and important new phenomenon in thin film science.

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C. Detavernier, A.S. Özcan, J. Jordan-Sweet, E.A. Stach, J. Tersoff, F.M. Ross, C. Lavoie; *An off-normal fiber-like texture in thin films on single crystalline substrates*, Nature, **426**, 641-5, 2003.